

# Claims

1. A method for routine determination of  $IC_{50}$  or  $EC_{50}$  values for compounds via biological assay at a single concentration, which comprises:
  - 5 a) Identifying a biological assay capable of producing a percent effect for a compound tested for activity against a target at a known concentration;
  - b) Performing the assay on an initial collection of at least 10 compounds, and at least 1 commercially available compound to be used as positive control, each assayed at a set of 3 to 10 or more concentrations, measuring a  
10 percent effect at each concentration for each compound;
  - c) Determining an  $IC_{50}$  or  $EC_{50}$  for each of these initial compounds by fitting a mathematical dose response curve to the data for each compound, using a computer, and standard linear or nonlinear regression techniques;
  - d) Using the resultant data from these initial compounds to fit a  
15 mathematical relationship between the  $IC_{50}$  or  $EC_{50}$  values and the percent inhibition values at a single fixed concentration  $X$ ,
  - e) Using a computer, and standard linear or nonlinear regression techniques, developing an equation relating  $IC_{50}$  or  $EC_{50}$  to percent inhibition or percent response on all remaining and future test compounds, at the previously fixed  
20 single concentration  $X$ , and determining the  $IC_{50}$  or  $EC_{50}$  via the mathematical equation developed in step d).
2. The method of claim 1 wherein said mathematical dose response curve is the Hill function,
$$percent\ inhibition = \frac{100}{1 + \left( \frac{IC_{50}}{concentration} \right)^h}$$
- 25 3. The method of claim 1 wherein said mathematical relationship is  $IC_{50} = \exp\{a + b \cdot (\text{percent inhibition at concentration } X)\}$ .
4. The method of claim 1 wherein said biological assay is an assay for drug-drug interactions related to the target cytochrome P450 (CYP).

5. The method of claim 4 wherein the target is selected from the group consisting of CYP2C9, CYP2D6, CYP3A4, CYP1A2, and CYP2C19.

6. The method of claim 1 where the target is an enzyme.

7. The method of claim 1 wherein the target is a receptor.

5 8. The method of claim 1 wherein the target is a transporter.

9. The method of claim 1 wherein said biological assay relates to affinity for any target protein wherein modulation of activity is therapeutically desired.

10. The method of claim 1 wherein said biological assay relates to affinity for any nontherapeutic protein wherein modulation of said activity is  
10 undesirable.